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## Lewis acid catalysis of a Diels-Alder reaction in water

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Supplementary material to:

**Lewis-Acid Catalysis of a Diels-Alder reaction in water.**

Sijbren Otto, Federica Bertoncin and Jan B. F. N. Engberts

Second-order rate constants ( $\text{M}^{-1}\text{s}^{-1}$ ) of the  $\text{Cu}^{2+}$ -catalyzed DA reaction of **1a**, **1b**, **1d** and **1e** with **2** in different solvents at 25°C.

Solvent	<b>1a</b>	<b>1b</b>	<b>1d</b>	<b>1e</b>
acetonitrile	2.21	0.594	0.240	0.0689
ethanol	0.769 <sup>a</sup>	0.382	0.162	0.0510
water	3.25	1.23	0.654	0.262
2,2,2-trifluoroethanol	15.6	3.31	1.52	0.549

(a) This value deviates from the otherwise linear Hammett-plot. In the Hammett correlation the rate constant for **1** with  $\text{X}=\text{CO}_2\text{CH}_3$  ( $k_2=0.655 \text{ M}^{-1}\text{s}^{-1}$ ) was used instead.

Equilibrium constants from complexation of **1a**, **1b**, **1d** and **1e** with different metal ions ( $K_a$ ) and second-order rate constants for the DA reaction of these complexes with **2** ( $k_2$ ) in water at 2.00 M ionic strength and 25°C.

	$\text{Co}^{2+}$		$\text{Ni}^{2+}$		$\text{Cu}^{2+}$		$\text{Zn}^{2+}$	
	$K_a$	$k_2$	$K_a$	$k_2$	$K_a$	$k_2$	$K_a$	$k_2$
<b>1a</b>	86.9	$2.84 \cdot 10^{-1}$	318	$5.69 \cdot 10^{-1}$	425	11.1	34.5	$5.03 \cdot 10^{-1}$
<b>1b</b>	112	$1.02 \cdot 10^{-1}$	579	$1.18 \cdot 10^{-1}$	1059	2.82	57.3	$1.22 \cdot 10^{-1}$
<b>1d</b>	127	$4.67 \cdot 10^{-2}$	947	$4.61 \cdot 10^{-2}$	1553	1.36	88.1	$5.81 \cdot 10^{-2}$
<b>1e</b>	178	$2.11 \cdot 10^{-2}$	1496	$1.91 \cdot 10^{-2}$	2759	0.518	161	$2.48 \cdot 10^{-2}$